# Shannon entropy and Fisher information for atoms in molecules

Chunying Rong,[1] Tian Lu,[2] and Shubin Liu [1,3*]

[1] *Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research (Ministry of Education of China) and Key Laboratory of Resource Fine-Processing and Advanced Materials of Hunan Province, College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha Hunan 410081, China*

[2] *School of Chemical and Biological Engineering, University of Science and Technology Beijing, Beijing, China*

[3] *Research Computing Center, University of North Carolina, Chapel Hill, North Carolina 27599-3420, U.S.A.*

**Abstract**

Shannon entropy and Fisher information are key quantities in information theory. Earlier, we have proved that these two quantities are intrinsically correlated for molecular systems.[1] Meanwhile, we recently proposed to use the Weizsäcker kinetic energy,[2] which differs from Fisher information by only a factor of 1/8, as a measure of the steric effect. These quantities involve only the electron density and its gradient, so, according to density functional theory, they are natural descriptors of a molecular system and thus should be able to determine all its properties including chemical reactivity.[3] In this work, we investigate these quantities from the perspective of density functional reactivity theory at both molecular and atomic levels. To that end, a new basin-based integration algorithm has been implemented,[4] whose reliability and effectiveness have been extensively examined. Interesting changing patterns for the atomic and molecular values of these quantities have been observed for different systems including bond stretching, bending, and rotating.[5] This work not only confirms the strong correlation between Shannon entropy and Fisher information for molecular species, as theoretically proven earlier by us, it also provides new and unexpected changing patterns for atomic values of these information-theoretic quantities, which can be employed to understand the origin and nature of chemical phenomena.[6]

**References**:

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